A Bayesian-motivated test for linear model in high-dimensional setting

Rui Wang

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1 Introduction

The proposed test is the limit of Bayes factors.

Fixed design

Suppose we would like to test the hypotheses:

$$\begin{aligned} \mathcal{H}_0 : \mathbf{y} &= \mathbf{X}_a\boldsymbol{\beta}_a + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}_n(0, \phi^{-1}\mathbf{I}_n), \\ \mathcal{H}_1 : \mathbf{y} &= \mathbf{X}_a\boldsymbol{\beta}_a + \mathbf{X}_b\boldsymbol{\beta}_b + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}_n(0, \phi^{-1}\mathbf{I}_n). \end{aligned}$$

Here $\boldsymbol{\beta}_a$ is q dimensional and $\boldsymbol{\beta}_b$ is p dimensional. We assume that as n tends to infinity, q is fixed while $p/n \to \infty$. This assumption is reasonable. We assume $\mathbf{X}_a$ has full column rank and $\mathbf{X}_b$ has full row rank. In practice, p_0 is often 1 and $\mathbf{X}_a$ is $\mathbf{1}_n$.

As Goeman et al. (2006) pointed out, if $\boldsymbol{\beta}_b \neq 0$ but $\mathbf{X}_b\boldsymbol{\beta}_b = 0$, no test has any power. Goeman et al. (2006) used Bayesian method. Their idea is to choose an 'unbiased' distribution of $\boldsymbol{\beta}_b$. As they noticed, their test has negligible power for many alternatives, and is not unbiased.

The following proposition implies that there is no nontrivial unbiased test.

Proposition 1. *Suppose $\mathbf{y} \sim \mathcal{N}_n(\mu, \phi^{-1}\mathbf{I}_n)$. We test $H_0 : \mu = \mathbf{X}_a\boldsymbol{\beta}_a, \boldsymbol{\beta}_a \in \mathbb{R}^q$ versus $H_1 : \mu \in \mathbb{R}^n$, where $\mathbf{X}_a$ is an $n \times q$ matrix with full column rank, $q < n$. Let $\varphi(\mathbf{y})$ be a test function, that is, a Borel measurable function, $0 \leq \phi(\mathbf{y}) \leq 1$. If $\int \varphi(\mathbf{y})\mathcal{N}_n(\mathbf{X}_a\boldsymbol{\beta}_a, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) = \alpha$ for $\boldsymbol{\beta}_a \in \mathbb{R}^q$, $\phi > 0$ and $\int \varphi(\mathbf{y})\mathcal{N}_n(\mu, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) \geq \alpha$ for $\mu \in \mathbb{R}^n$, $\phi > 0$, then $\varphi(\mathbf{y}) = \alpha$, a.s.*

So we can not find a universally good test. Instead, we would like to find a test with good average behaviour. So Bayesian methods are natural choices in this case.

Bayes hypothesis testing use the Bayes factor.

$$B_{10} = \frac{\int f_1(\mathbf{y}|\boldsymbol{\beta}_b, \boldsymbol{\beta}_a, \phi)\pi_1(\boldsymbol{\beta}_b, \boldsymbol{\beta}_a, \phi)d\boldsymbol{\beta}_b d\boldsymbol{\beta}_a d\phi}{\int f_0(\mathbf{y}|\boldsymbol{\beta}_a, \phi)\pi_0(\boldsymbol{\beta}_a, \phi)d\boldsymbol{\beta}_a d\phi}.$$

There have been several extensions of g-priors to $p > n$ case: Maruyama and George (2011), Shang and Clayton (2011).

Under H_0, we impose the reference prior $\pi_0(\boldsymbol{\beta}_a, \phi) = c/\phi$. Note that under H_1, the posterior corresponding to the referece prior is proper if and only if $\text{Rank}(\mathbf{X}_a, \mathbf{X}_b) = q + p$ and $n > q + p$. That is, the minimal training sample size is $q+p+1$. So we cannot impose the reference prior under H_1 provided $q + p \geq n$. We temporarily impose the conditional prior $\boldsymbol{\beta}_b|\boldsymbol{\beta}_a, \phi \sim \mathcal{N}_p(0, \kappa^{-1}\phi^{-1}\mathbf{I}_p)$. There are extansive literature consider the choice of κ. Kass and Wasserman (1995) choose κ such that the amount of information about the parameter equal to the amount of information contained in one observation. Thus, under H_1, we put the prior

$$\pi_1(\boldsymbol{\beta}_b|\boldsymbol{\beta}_a, \phi) = \mathcal{N}_p\left(0, \frac{1}{\kappa\phi}\mathbf{I}_p\right)(\boldsymbol{\beta}_b), \quad \pi_1(\boldsymbol{\beta}_a, \phi) = \frac{c}{\phi}.$$

$$\begin{aligned} m_0(\mathbf{y}; \kappa, \tau) &:= \int f_0^\tau(\mathbf{y}|\boldsymbol{\beta}_a, \phi)\pi_0(\boldsymbol{\beta}_a, \phi)d\boldsymbol{\beta}_a d\phi \\ &= \frac{c_0\Gamma\left(\frac{\tau n - q}{2}\right)}{\pi^{\frac{\tau n - q}{2}}\tau^{\frac{\tau n}{2}}|\mathbf{X}_a^\top\mathbf{X}_a|^{\frac{1}{2}}\|(\mathbf{I}_n - \mathbf{P}_a)\mathbf{y}\|^{\tau n - q}}. \end{aligned}$$

$$\begin{aligned} m_1(\mathbf{y}; \kappa, \tau) &:= \int f_1^\tau(\mathbf{y}|\boldsymbol{\beta}_b, \boldsymbol{\beta}_a, \phi)\pi_1(\boldsymbol{\beta}_b|\boldsymbol{\beta}_a, \phi)\pi_1(\boldsymbol{\beta}_a, \phi)d\boldsymbol{\beta}_a d\boldsymbol{\beta}_b d\phi \\ &= \frac{c_1\kappa^{\frac{p}{2}}\Gamma\left(\frac{\tau n - q}{2}\right)}{\pi^{\frac{\tau n - q}{2}}\tau^{\frac{\tau n + p}{2}}|\mathbf{X}_a^\top\mathbf{X}_a|^{\frac{1}{2}}|\mathbf{X}_b^{*\top}\mathbf{X}_b^* + \frac{\kappa}{\tau}\mathbf{I}_p|^{\frac{1}{2}}} \frac{1}{\left[\mathbf{y}^{*\top}\mathbf{y}^* - \mathbf{y}^{*\top}\mathbf{X}_b^*(\mathbf{X}_b^{*\top}\mathbf{X}_b^* + \frac{\kappa}{\tau}\mathbf{I}_p)^{-1}\mathbf{X}_b^{*\top}\mathbf{y}^*\right]^{\frac{\tau n - q}{2}}}. \end{aligned}$$

$$\frac{m_1(\mathbf{y}; \kappa, \tau)}{m_0(\mathbf{y}; \kappa, \tau)} = \frac{c_1\kappa^{\frac{p}{2}}}{c_0\tau^{\frac{p}{2}}|\mathbf{X}_b^{*\top}\mathbf{X}_b^* + \frac{\kappa}{\tau}\mathbf{I}_p|^{\frac{1}{2}}}\left(\frac{\mathbf{y}^{*\top}\mathbf{y}^*}{\mathbf{y}^{*\top}\mathbf{y}^* - \mathbf{y}^{*\top}\mathbf{X}_b^*(\mathbf{X}_b^{*\top}\mathbf{X}_b^* + \frac{\kappa}{\tau}\mathbf{I}_p)^{-1}\mathbf{X}_b^{*\top}\mathbf{y}^*}\right)^{\frac{\tau n - q}{2}}$$

It is straightforward to show that the Bayes factor associated with these priors is

$$\begin{aligned} B_{10}^\kappa =& \frac{\kappa^{p/2}}{|\mathbf{X}_b^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b + \kappa\mathbf{I}_p|^{1/2}} \cdot \\ & \left(\frac{\mathbf{y}\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{y}}{\mathbf{y}\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{y} - \mathbf{y}\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b\left(\mathbf{X}_b^\top(\mathbf{I} - \mathbf{P}_a)\mathbf{X}_b + \kappa\mathbf{I}_p\right)^{-1}\mathbf{X}_b^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{y}}\right)^{(n-q)/2}. \end{aligned}$$

Thus,

$$\begin{aligned} 2\log B_{10}^\kappa =& p\log\kappa - \log|\mathbf{X}_b^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b + \kappa\mathbf{I}_p| \\ & - (n - q)\log\left(1 - \frac{\mathbf{y}\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b\left(\mathbf{X}_b^\top(\mathbf{I} - \mathbf{P}_a)\mathbf{X}_b + \kappa\mathbf{I}_p\right)^{-1}\mathbf{X}_b^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{y}}{\mathbf{y}\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{y}}\right). \end{aligned}$$

Denote by $\mathbf{I}_n - \mathbf{P}_a = \tilde{\mathbf{U}}_a\tilde{\mathbf{U}}_a^\top$ the rank decomposition of $\mathbf{I}_n - \mathbf{P}_a$, where $\tilde{\mathbf{U}}_a$ is a $n \times (n - q)$ column orthogonal matrix. Let $\mathbf{X}_b^* = \tilde{\mathbf{U}}_a^\top\mathbf{X}_b$, $\mathbf{y}^* = \tilde{\mathbf{U}}_a^\top\mathbf{y}$. Let γ_i be the ith largest eigenvalue of $\mathbf{X}_b^*\mathbf{X}_b^{*\top}$, $i = 1, \ldots, n - q$. Denote by $\mathbf{X}_b^* = \mathbf{U}_b^*\mathbf{D}_b^*\mathbf{V}_b^{*\top}$ the singular value decomposition of $\mathbf{X}_b^*$, where $\mathbf{U}_b^*$, $\mathbf{V}_b^*$ are $(n - q) \times (n - q)$ and $p \times (n - q)$ column orthogonal matrices, respectively, and $\mathbf{D}_b^* = \text{diag}(\sqrt{\gamma_1}, \ldots, \sqrt{\gamma_{n-q}})$. Then

$$
\begin{aligned}
2\log B_{10}^{\kappa} =& p\log\kappa - \sum_{i=1}^{n-q}\log(\gamma_i+\kappa) - (p-(n-q))\log\kappa \\
& - (n-q)\log\left(1 - \frac{\mathbf{y}^{*\top}\mathbf{X}_b^{*}\left(\mathbf{X}_b^{*\top}\mathbf{X}_b^{*}+\kappa\mathbf{I}_p\right)^{-1}\mathbf{X}_b^{*\top}\mathbf{y}^{*}}{\mathbf{y}^{*\top}\mathbf{y}^{*}}\right) \\
=& -\sum_{i=1}^{n-q}\log(\gamma_i+\kappa) + (n-q)\log\left(\frac{\mathbf{y}^{*\top}\mathbf{y}^{*}}{\mathbf{y}^{*\top}\mathbf{U}_b^{*}\left[\frac{1}{\kappa}\left(\mathbf{I}_{n-q}-\mathbf{D}_b^{*}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*}\right)\right]\mathbf{U}_b^{*\top}\mathbf{y}^{*}}\right) \\
=& (n-q)\log\kappa - \sum_{i=1}^{n-q}\log(\gamma_i+\kappa) - (n-q)\log\left(1 - \frac{\mathbf{y}^{*\top}\mathbf{U}_b^{*}\mathbf{D}_b^{*}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*}\mathbf{U}_b^{*\top}\mathbf{y}^{*}}{\mathbf{y}^{*\top}\mathbf{y}^{*}}\right).
\end{aligned}
$$

The main part of $2\log B_{10}^{\kappa}$ is

$$
T_n^{\kappa} = \frac{\mathbf{y}^{*\top}\mathbf{U}_b^{*}\mathbf{D}_b^{*}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*}\mathbf{U}_b^{*\top}\mathbf{y}^{*}}{\mathbf{y}^{*\top}\mathbf{y}^{*}}.
$$

A large value of T_n^{κ} supports the alternative hypothesis. Under the null hypothesis,

$$
\mathrm{E}\,T_n^{\kappa} = \frac{1}{n-q}\operatorname{tr}\left(\mathbf{D}_b^{*2}(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q})^{-1}\right).
$$

Under the alternative hypothesis, consider $\boldsymbol{\beta}_b = c\boldsymbol{\beta}_b^{\dagger}$ where $\boldsymbol{\beta}_b^{\dagger}\neq 0$ is a fixed direction and $c>0$. As $c\to\infty$,

$$
T_n^{\kappa} \to \frac{\boldsymbol{\beta}_b^{\dagger\top}\mathbf{V}_b^{*}\mathbf{D}_b^{*2}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*2}\mathbf{V}_b^{*\top}\boldsymbol{\beta}_b^{\dagger}}{\boldsymbol{\beta}_b^{\dagger\top}\mathbf{V}_b^{*}\mathbf{D}_b^{*2}\mathbf{V}_b^{*\top}\boldsymbol{\beta}_b^{\dagger}}.
$$

We say T_n^{κ} is consistent along the direction $\boldsymbol{\beta}_b^{\dagger}$ if

$$
\frac{\boldsymbol{\beta}_b^{\dagger\top}\mathbf{V}_b^{*}\mathbf{D}_b^{*2}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*2}\mathbf{V}_b^{*\top}\boldsymbol{\beta}_b^{\dagger}}{\boldsymbol{\beta}_b^{\dagger\top}\mathbf{V}_b^{*}\mathbf{D}_b^{*2}\mathbf{V}_b^{*\top}\boldsymbol{\beta}_b^{\dagger}} > \frac{1}{n-q}\operatorname{tr}\left(\mathbf{D}_b^{*2}(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q})^{-1}\right),
$$

or equivalently

$$
\boldsymbol{\beta}_b^{\dagger\top}\mathbf{V}_b^{*}\left[\mathbf{D}_b^{*2}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*2} - \frac{1}{n-q}\operatorname{tr}\left(\mathbf{D}_b^{*2}(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q})^{-1}\right)\mathbf{D}_b^{*2}\right]\mathbf{V}_b^{*\top}\boldsymbol{\beta}_b^{\dagger} > 0.
$$

Let k_{κ} be the number of positive eigenvalues of

$$
\mathbf{V}_b^{*}\left[\mathbf{D}_b^{*2}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*2} - \frac{1}{n-q}\operatorname{tr}\left(\mathbf{D}_b^{*2}(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q})^{-1}\right)\mathbf{D}_b^{*2}\right]\mathbf{V}_b^{*\top}.
$$

Let $\mathcal{S}_{\kappa}$ be the linear space spanned by the first k_{κ} columns of $\mathbf{V}_b^{*}$. Denote by $\mathcal{S}_{\kappa}^{\perp}$ the orthogonal complement space of $\mathcal{S}_{\kappa}$. We have $\mathbb{R}^p = \mathcal{S}_{\kappa}\oplus\mathcal{S}_{\kappa}^{\perp}$. If $\boldsymbol{\beta}_b^{\dagger}\in\mathcal{S}_{\kappa}$,

$$
\mathbf{V}_b^{*}\left[\mathbf{D}_b^{*2}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*2} - \frac{1}{n-q}\operatorname{tr}\left(\mathbf{D}_b^{*2}(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q})^{-1}\right)\mathbf{D}_b^{*2}\right]\mathbf{V}_b^{*\top} > 0.
$$

On the other hand, if $\boldsymbol{\beta}_b^\dagger \in \mathcal{S}_\kappa^\perp$,

$$\mathbf{V}_b^* \left[\mathbf{D}_b^{*2}\left(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q}\right)^{-1}\mathbf{D}_b^{*2} - \frac{1}{n-q}\operatorname{tr}\left(\mathbf{D}_b^{*2}(\mathbf{D}_b^{*2}+\kappa\mathbf{I}_{n-q})^{-1}\right)\mathbf{D}_b^{*2}\right]\mathbf{V}_b^{*\top} \leq 0.$$

We would like to choose a hyperparameter κ which consists the most consistent directions. To achieve this, we maximize k_κ with respect to κ.

Proposition 2. *For $\kappa_2 > \kappa_1 > 0$, we have $k_{\kappa_1} \geq k_{\kappa_2}$. That is, k_κ ($\kappa > 0$) is decreasing in κ.*

The proposition implies that we should put κ as small as possible. This motivates us to consider $B_{10}^0 = \lim_{\kappa\to 0} B_{10}^\kappa$. It is straightforward to show that

$$2\log B_{10}^0 = -\sum_{i=1}^{n-q}\log(\gamma_i) + (n-q)\log\left(\frac{\mathbf{y}^{*\top}\mathbf{y}^*}{\mathbf{y}^{*\top}(\mathbf{X}_b^*\mathbf{X}_b^{*\top})^{-1}\mathbf{y}^*}\right).$$

B_{10}^0 can be regarded as the Bayes factor with respect to noninformative prior.

Define

$$T_n = \frac{\mathbf{y}^{*\top}(\mathbf{X}_b^*\mathbf{X}_b^{*\top})^{-1}\mathbf{y}^*}{\mathbf{y}^{*\top}\mathbf{y}^*}.$$

Then we reject the null hypothesis if T_n is small. It can be seen that under the null hypohtesis,

$$T_n \sim \frac{\sum_{i=1}^{n-q}\gamma_i^{-1}Z_i^2}{\sum_{i=1}^{n-q}Z_i^2},$$

where γ_i is the ith eigenvalue of $\mathbf{X}_b^*\mathbf{X}_b^{*\top}$, $i = 1, \ldots, n-q$, and $Z_1, \ldots, Z_{n-q}$ are iid $\mathcal{N}(0,1)$ random variables.

2 Asymptotic results

Let $\boldsymbol{\varepsilon} = (\epsilon_1, \ldots, \epsilon_n)^\top$, where ϵ_i's are iid random variable. Denote $\mu_k = \operatorname{E}\epsilon_1^k$. Then $\mu_1 = 0$, $\mu_2 = \phi^{-1}$.

Lemma 1. *If $\phi^2\mu_4 = o(n-q)$,*

$$\mathbf{y}^{*\top}\mathbf{y}^* = (1+o_P(1))\left(\boldsymbol{\beta}_b^\top\mathbf{X}_b^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b\boldsymbol{\beta}_b + \phi^{-1}(n-q)\right).$$

Proof.

$$\mathbf{y}^{*\top}\mathbf{y}^* = \boldsymbol{\beta}_b^\top\mathbf{X}_b^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b\boldsymbol{\beta}_b + 2\boldsymbol{\varepsilon}^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b\boldsymbol{\beta}_b + \boldsymbol{\varepsilon}^\top(\mathbf{I}_n - \mathbf{P}_a)\boldsymbol{\varepsilon}.$$

$$\operatorname{E}\left(\mathbf{y}^{*\top}\mathbf{y}^*\right) = \boldsymbol{\beta}_b^\top\mathbf{X}_b^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b\boldsymbol{\beta}_b + \phi^{-1}(n-q).$$

$$\operatorname{Var}\left(\mathbf{y}^{*\top}\mathbf{y}^*\right) \leq 2\operatorname{Var}\left(2\boldsymbol{\varepsilon}^\top(\mathbf{I}_n - \mathbf{P}_a)\mathbf{X}_b\boldsymbol{\beta}_b\right) + 2\operatorname{Var}\left(\boldsymbol{\varepsilon}^\top(\mathbf{I}_n - \mathbf{P}_a)\boldsymbol{\varepsilon}\right)$$

From (i) of (Chen et al., 2010, Proposition A.1),

$$\operatorname{Var}\left(\boldsymbol{\varepsilon}^\top(\mathbf{I}_n-\mathbf{P}_a)\boldsymbol{\varepsilon}\right)=\phi^{-2}\left((\phi^2\mu_4-3)\sum_{i=1}^n((\mathbf{I}_n-\mathbf{P}_a)_{i,i})^2+2(n-q)\right)\leq\phi^{-2}(2+\phi^2\mu_4)(n-q).$$

Then

$$\operatorname{Var}\left(\mathbf{y}^{*\top}\mathbf{y}^*\right)\leq 8\phi^{-1}\boldsymbol{\beta}_b^\top\mathbf{X}_b^\top(\mathbf{I}_n-\mathbf{P}_a)\mathbf{X}_b\boldsymbol{\beta}_b+2\phi^{-2}(2+\phi^2\mu_4)(n-q)$$

Thus, if $\phi^2\mu_4=o(n-q)$, we have

$$\frac{\operatorname{Var}\left(\mathbf{y}^{*\top}\mathbf{y}^*\right)}{\left(\operatorname{E}\left(\mathbf{y}^{*\top}\mathbf{y}^*\right)\right)^2}\to 0,$$

and consequently $\mathbf{y}^{*\top}\mathbf{y}^*=(1+o_P(1))\operatorname{E}(\mathbf{y}^{*\top}\mathbf{y}^*)$.

□

Note that under the normality, $T_n-\operatorname{tr}((\mathbf{X}_b^*\mathbf{X}_b^{*\top})^{-1})/(n-q)$ has zero mean.

Theorem 1. *Let $\mathbf{A}_n$ be an $(n-q)\times(n-q)$ symmetric matrix.*

$$\left(\boldsymbol{\beta}_b^\top\mathbf{X}_b^\top(\mathbf{I}_n-\mathbf{P}_a)\mathbf{X}_b\boldsymbol{\beta}_b+\phi^{-1}(n-q)\right)\left(\frac{\mathbf{y}^{*\top}\mathbf{A}_n\mathbf{y}^*}{\mathbf{y}^{*\top}\mathbf{y}^*}-\frac{\operatorname{tr}(\mathbf{A}_n)}{n-q}\right)\rightsquigarrow\mathcal{N}(0,1).$$

Proof.

$$\frac{\mathbf{y}^{*\top}\mathbf{A}_n\mathbf{y}^*}{\mathbf{y}^{*\top}\mathbf{y}^*}-\frac{\operatorname{tr}(\mathbf{A}_n)}{n-q}=\frac{\mathbf{y}^\top\left(\tilde{\mathbf{U}}_a\mathbf{A}_n\tilde{\mathbf{U}}_a^\top-\frac{\operatorname{tr}(\mathbf{A}_n)}{n-q}\tilde{\mathbf{U}}_a\tilde{\mathbf{U}}_a^\top\right)\mathbf{y}}{\mathbf{y}^{*\top}\mathbf{y}^*}.$$

123

From (Jiang, 1996, Theorem 5.1), □

Appendices

Appendix A haha1

Proof of Proposition 1. We assume $0<\alpha<1$ since the case $\alpha=0$ or 1 is trivial. Note that the condition implies $\int[\varphi(\mathbf{y})-\alpha]\mathcal{N}_n(0,\phi^{-1}\mathbf{I}_n)(d\mathbf{y})=0$. Hence it suffices to prove $\varphi(\mathbf{y})\geq\alpha$, a.s. We prove this by contradiction. Suppose $\lambda(\{\mathbf{y}:\varphi(\mathbf{y})<\alpha\})>0$. Then there exists a $\eta>0$, such that $\lambda(\{\mathbf{y}:\varphi(\mathbf{y})<\alpha-\eta\})>0$. We denote $E=\{\mathbf{y}:\varphi(\mathbf{y})<\alpha-\eta\}$. From Lebesgue density theorem (Cohn, 2013, Corollary 6.2.6), there exists a point $z\in E$, such that, for each $\epsilon>0$ there is a $\delta_\epsilon>0$ such that

$$\left|\frac{\lambda(E^\complement\cap C_\epsilon)}{\lambda(C_\epsilon)}\right|<\epsilon,$$

where $C_\epsilon = \prod_{i=1}^n [z_i - \delta_\epsilon, z_i + \delta_\epsilon]$. We put

$$\epsilon = \left(\frac{\sqrt{\pi}}{\sqrt{2}\Phi^{-1}\left(1 - \frac{\eta}{6n}\right)} \right)^n \frac{\eta}{3}.$$

Then for any $\phi > 0$,

$$\begin{aligned}
\alpha \leq& \int_{\mathbb{R}^n} \varphi(\mathbf{y}) \mathcal{N}_n(z, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) \\
=& \int_{E \cap C_\epsilon} \varphi(\mathbf{y}) \mathcal{N}_n(z, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) + \int_{E^\complement \cap C_\epsilon} \varphi(\mathbf{y}) \mathcal{N}_n(z, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) + \int_{C_\epsilon^\complement} \varphi(\mathbf{y}) \mathcal{N}_n(z, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) \\
\leq& \alpha - \eta + \int_{E^\complement \cap C_\epsilon} \mathcal{N}_n(z, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) + \int_{C_\epsilon^\complement} \mathcal{N}_n(z, \phi^{-1}\mathbf{I}_n)(d\mathbf{y}) \\
\leq& \alpha - \eta + \left(\frac{\phi}{2\pi} \right)^{n/2} \lambda(E^\complement \cap C_\epsilon) + 2n \left(1 - \Phi(\sqrt{\phi}\delta_\epsilon) \right) \\
\leq& \alpha - \eta + \left(\frac{\phi}{2\pi} \right)^{n/2} \epsilon (2\delta_\epsilon)^n + 2n \left(1 - \Phi(\sqrt{\phi}\delta_\epsilon) \right) \\
=& \alpha - \eta + \left(\frac{\sqrt{\phi}\delta_\epsilon}{\Phi^{-1}\left(1 - \frac{\eta}{6n}\right)} \right)^n \frac{\eta}{3} + 2n \left(1 - \Phi(\sqrt{\phi}\delta_\epsilon) \right).
\end{aligned}$$

Putting

$$\phi = \left(\frac{\Phi^{-1}\left(1 - \frac{\eta}{6n}\right)}{\delta_\epsilon} \right)^2$$

yields the contradiction $\alpha \leq \alpha - (2/3)\eta$. This completes the proof.

□

Proof of Proposition 2. For positive integer m, define $[m] = \{1, , \ldots, m\}$. For a set A, denote by $|A|$ its cardinality. We have

$$\begin{aligned}
k_\kappa =& \left| \left\{ i \in [n-q] : \frac{\gamma_i^2}{\gamma_i + \kappa} - \frac{1}{n-q} \sum_{j=1}^{n-q} \frac{\gamma_j \gamma_i}{\gamma_j + \kappa} > 0 \right\} \right| \\
=& \left| \left\{ i \in [n-q] : \frac{\gamma_i}{\gamma_i + \kappa} > \frac{1}{n-q} \sum_{j=1}^{n-q} \frac{\gamma_j}{\gamma_j + \kappa} \right\} \right|.
\end{aligned}$$

Let X be a random variable uniformly distributed on $\{\gamma_1, \ldots, \gamma_{n-q}\}$. That is, $\Pr(X = \gamma_i) = 1/(n-q)$, $i = 1, \ldots, n-q$. Then it can be seen that

$$k_\kappa = (n-q) \Pr\left(\frac{X}{X+\kappa} > \mathrm{E}\left[\frac{X}{X+\kappa} \right] \right).$$

Hence we only need to verify

$$\Pr\left(\frac{X}{X+\kappa_1} > \mathrm{E}\left[\frac{X}{X+\kappa_1} \right] \right) \geq \Pr\left(\frac{X}{X+\kappa_2} > \mathrm{E}\left[\frac{X}{X+\kappa_2} \right] \right). \tag{1}$$

Let $Y = X/(X+\kappa_2)$. Then

$$\frac{X}{(X+\kappa_1)} = \frac{\kappa_2 Y}{\kappa_1 + (\kappa_2 - \kappa_1)Y} := f(Y).$$

Note that $f(Y)$ is increasing for $Y \geq 0$. Then the inequality (1) is equivalent to

$$\Pr\left(Y > f^{-1}\left(\operatorname{E} f(Y)\right)\right) \geq \Pr\left(Y > \operatorname{E} Y\right).$$

Hence we only need to verify $f^{-1}\left(\operatorname{E} f(Y)\right) \leq \operatorname{E} Y$, or equivalently, $\operatorname{E} f(Y) \leq f(\operatorname{E} Y)$. But the last inequality is a direct consequence of the concavity of $f(Y)$. This completes the proof.

□

Appendix B haha2

Theorem 2. *Let $\zeta_1, \ldots, \zeta_d$ be iid random variables with mean 0 and variance 1, and assume $\mu_k := \operatorname{E}(\zeta_1^k)$ is finite for $k \leq 8$. Let $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_d)^\top \in \mathbb{R}^d$. For $k = 1, \ldots, K$, let $\mathbf{Q}_k = (q_{i_j}^{(k)})$ be a $d \times d$ symmetric matrix and let $\check{\mathbf{Q}}_k = \operatorname{diag}(q_{11}^{(k)}, \ldots, q_{dd}^{(k)})$, $\hat{\mathbf{Q}}_k = \mathbf{I}_d - \check{\mathbf{Q}}_k$. Define $\hat{w}_k = \boldsymbol{\zeta}^\top \hat{\mathbf{Q}}_k \boldsymbol{\zeta}$, $\check{w}_k = \boldsymbol{\zeta}^\top \check{\mathbf{Q}}_k \boldsymbol{\zeta} - \operatorname{tr}(\mathbf{Q}_k)$, and*

$$W = \begin{pmatrix} \hat{w}_1 \\ \check{w}_1 \\ \vdots \\ \hat{w}_K \\ \check{w}_K \end{pmatrix} = \begin{pmatrix} \boldsymbol{\zeta}^\top \hat{\mathbf{Q}}_1 \boldsymbol{\zeta} \\ \boldsymbol{\zeta}^\top \check{\mathbf{Q}}_1 \boldsymbol{\zeta} - \operatorname{tr}(\mathbf{Q}_1) \\ \vdots \\ \boldsymbol{\zeta}^\top \hat{\mathbf{Q}}_1 \boldsymbol{\zeta} \\ \boldsymbol{\zeta}^\top \check{\mathbf{Q}}_1 \boldsymbol{\zeta} - \operatorname{tr}(\mathbf{Q}_1) \end{pmatrix} \in \mathbb{R}^{2K}.$$

Finally, let $Z \sim \mathcal{N}_{2K}(0, \mathbf{I}_{2K})$ and $\mathbf{V} = \operatorname{Cov}(W)$. There is an absolute constant $0 < C < \infty$ such that

haha

Proof. Let $f : \mathbb{R}^{2K} \to \mathbb{R}$ be a four-times differentiable function. From xxx, there is a $4-times$ differentiable function $g : \mathbb{R}^{2K} \to \mathbb{R}$ satisfying the Stein identity

$$\operatorname{E}[f(W)] - \operatorname{E}[f(\mathbf{V}^{1/2}W)] = \operatorname{E}[\nabla^\top \mathbf{V} \nabla g(W) - W^\top \nabla g(W)]$$

and

$$\left|\frac{\partial^k g(\mathbf{x})}{\prod_{j=1}^k \partial x_{i_j}}\right| \leq \frac{1}{k}\left|\frac{\partial^k f(\mathbf{x})}{\prod_{j=1}^k \partial x_{i_j}}\right| \quad \text{for all } \mathbf{x} = (x_1, \ldots, x_{2K})^\top \in \mathbb{R}^{2K},\ k = 1,2,3, \text{ and } i_j \in \{1, \ldots, 2K\}.$$

To prove the theorem, we bound

$$S = \operatorname{E}[\nabla^\top \mathbf{V} \nabla g(W) - W^\top \nabla g(W)].$$

Next, we use exchangeability. Let $\boldsymbol{\zeta}' = (\zeta_1', \ldots, \zeta_d')^\top$ be an independent copy of ζ, and let $\underline{i} \in \{1, \ldots, d\}$ be an independent and uniformly distributed random index. Define the vector

$W' \in \mathbb{R}^{2K}$ exactly as we defined W, except that $\boldsymbol{\zeta}_{\underline{i}}$ is replaced with $\boldsymbol{\zeta}'_{\underline{i}}$ throughout. More precisely, let $e_i \in \mathbb{R}^d$ be the ith standard basis vector in $\mathcal{R}^d$ and define

$$\begin{aligned}\hat{w}'_k =&(\boldsymbol{\zeta} + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}})^\top \hat{\mathbf{Q}}_k(\boldsymbol{\zeta} + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}})\\ =&\hat{w}_k + 2(\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}}^\top \hat{\mathbf{Q}}_k\boldsymbol{\zeta},\end{aligned}$$

$$\begin{aligned}\check{w}'_k =&(\boldsymbol{\zeta} + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}})^\top \check{\mathbf{Q}}_k(\boldsymbol{\zeta} + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}}) - \operatorname{tr}(\mathbf{Q}_k)\\ =&\check{w}_k + e_{\underline{i}}^\top \check{\mathbf{Q}}_k e_{\underline{i}}((\zeta'_{\underline{i}})^2 - \zeta_{\underline{i}}^2),\end{aligned}$$

for $k = 1, \ldots, K$. Then $W' = (\hat{w}'_1, \check{w}'_1, \ldots, \hat{w}'_K, \check{w}'_K)^\top \in \mathbb{R}^{2K}$. Its straightforward to verify that

$$\mathrm{E}(\hat{w}'_k - \hat{w}_k|\boldsymbol{\zeta}) = -\frac{2}{d}\hat{w}_k, \quad \mathrm{E}(\check{w}'_k - \check{w}_k|\boldsymbol{\zeta}) = -\frac{1}{d}\check{w}_k.$$

Then

$$\mathrm{E}(W' - W|\boldsymbol{\zeta}) = -\Lambda_K W,$$

where

$$\Lambda_1 = \begin{pmatrix} \frac{2}{d} & 0 \\ 0 & \frac{1}{d} \end{pmatrix}, \quad \Lambda_K = \begin{pmatrix} \Lambda_1 & 0 & \cdots & 0 \\ 0 & \Lambda_1 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \Lambda_1 \end{pmatrix} \in \mathbb{R}^{2K \times 2K}.$$

By exchangeability, we have

$$\begin{aligned}0 =&\frac{1}{2}\,\mathrm{E}[(W' - W)^\top \Lambda_K^{-\top}(\nabla g(W') + \nabla g(W))]\\ =&\,\mathrm{E}[(W' - W)^\top \Lambda_K^{-\top}\nabla g(W)] + \frac{1}{2}\,\mathrm{E}[(W' - W)^\top \Lambda_K^{-\top}(\nabla g(W') - \nabla g(W))]\\ =&-\mathrm{E}[W^\top \nabla g(W)] + \frac{1}{2}\,\mathrm{E}[(W' - W)^\top \Lambda_K^{-\top}(\nabla g(W') - \nabla g(W))].\end{aligned}$$

That is,

$$\mathrm{E}[W^\top \nabla g(W)] = \frac{1}{2}\,\mathrm{E}[(W' - W)^\top \Lambda_K^{-\top}(\nabla g(W') - \nabla g(W))].$$

Apply Taylor's theorem,

$$\begin{aligned}&W^\top \nabla g(W)\\ =&\frac{1}{2}\sum_{i,j=1}^{2K} \Lambda_{K,ii}^{-1} D^{ij} g(W)(w'_i - w_i)(w'_j - w_j) + \frac{1}{4}\sum_{i,j,k=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijk} g(W)(w'_i - w_i)(w'_j - w_j)(w'_k - w_k)\\ &+ \frac{1}{12}\sum_{i,j,k,l=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijkl} g(t^*(W' - W) + W)(w'_i - w_i)(w'_j - w_j)(w'_k - w_k)(w'_l - w_l)\\ =&\frac{1}{2}\operatorname{tr}[(W' - W)(W' - W)^\top \Lambda_K^{-\top}\nabla^2 g(W)] + \frac{1}{4}\sum_{i,j,k=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijk} g(W)(w'_i - w_i)(w'_j - w_j)(w'_k - w_k)\\ &+ \frac{1}{12}\sum_{i,j,k,l=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijkl} g(t^*(W' - W) + W)(w'_i - w_i)(w'_j - w_j)(w'_k - w_k)(w'_l - w_l),\end{aligned} \tag{2}$$

where $t^* \in [0,1]$. Also by exchangeability,

$$\mathrm{E}[(W'-W)(W'-W)^\top] = 2\,\mathrm{E}[W(W-W')^\top] = 2\,\mathrm{E}[WW^\top\Lambda_K^\top] = 2\mathbf{V}\Lambda_K^\top.$$

It follows that

$$\mathrm{E}[\nabla^\top\mathbf{V}\nabla g(W)] = \mathrm{E}\,\mathrm{tr}[\mathbf{V}\nabla^2 g(W)] = \frac{1}{2}\,\mathrm{E}\,\mathrm{tr}[\mathrm{E}[(W'-W)(W'-W)^\top]\Lambda_K^{-\top}\nabla^2 g(W)]$$

Thus,

$$\begin{aligned}
S =& \mathrm{E}[\nabla^\top\mathbf{V}\nabla g(W) - W^\top\nabla g(W)] \\
=& \frac{1}{2}\,\mathrm{E}\,\mathrm{tr}[\mathrm{E}[(W'-W)(W'-W)^\top]\Lambda_K^{-\top}\nabla^2 g(W)] - \frac{1}{2}\,\mathrm{E}\,\mathrm{tr}[(W'-W)(W'-W)^\top\Lambda_K^{-\top}\nabla^2 g(W)] \\
& - \frac{1}{4}\,\mathrm{E}\sum_{i,j,k=1}^{2K}\Lambda_{K,ii}^{-1}D^{ijk}g(W)(w_i'-w_i)(w_j'-w_j)(w_k'-w_k) \\
& - \frac{1}{12}\,\mathrm{E}\sum_{i,j,k,l=1}^{2K}\Lambda_{K,ii}^{-1}D^{ijkl}g(t^*(W'-W)+W)(w_i'-w_i)(w_j'-w_j)(w_k'-w_k)(w_l'-w_l).
\end{aligned}$$

□

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